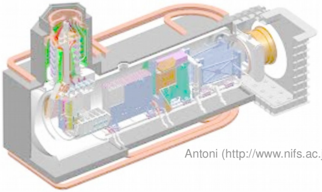
Improving computational efficiency of kinetic simulations with physics, mathematics, and machine learning

George J. Wilkie
National Research Institute for Mathematics and Computer Science (CWI)
Amsterdam, The Netherlands

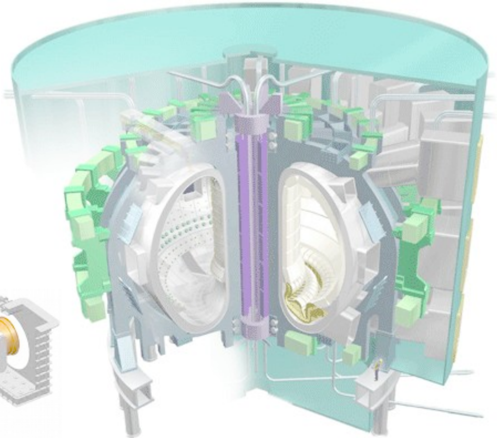
11 April 2019

PPPL theory seminar

Ashes to ashes: neutral gas to plasma and back again



Antoni (http://www.nifs.ac.jp)



http://www.itercad.org

Ashes to ashes: neutral gas to plasma and back again

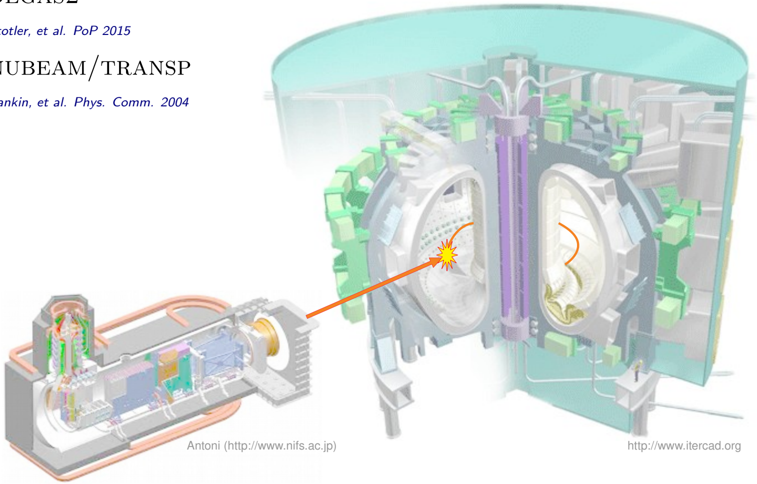
Neutral beam injection/ionization

- DEGAS2

  Stotler, et al. PoP 2015

- NUBEAM/TRANSP

  Pankin, et al. Phys. Comm. 2004



Ashes to ashes: neutral gas to plasma and back again

Alfvén eigenmodes

Fu & Van Dam. PoF-B. 1989

Cheng, Gorelenkov & Hsu. NF 1995

Berk, Breizman & Pekker. PRL 1996

Zonca, Chen & Santoro. PPCF 1996

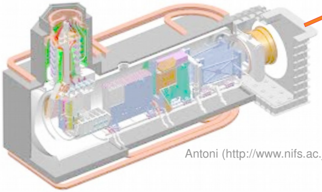
Schneller, et al. NF 2013

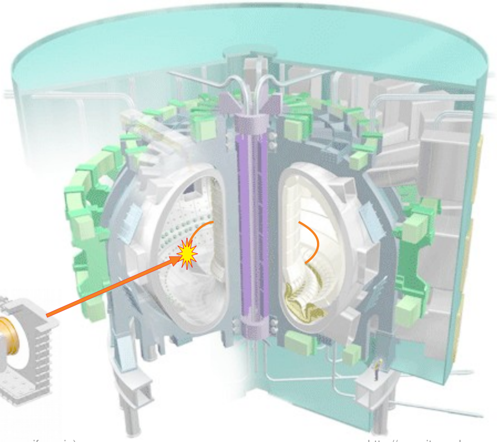
Duarte, et al. NF 2017

EGAMs

Fu. PRL 2008

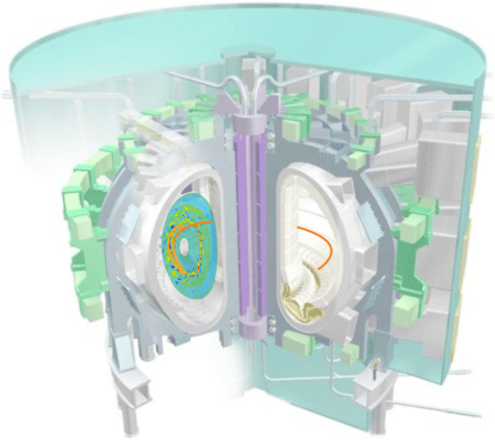
Berk & Zhou. NF 2010





Ashes to ashes: neutral gas to plasma and back again

Thermalization and turbulent transport



http://www.itercad.org
Görler, et al. PoP 2011

With precomputed diffusion coefficients, non-Maxwellian transport is greatly simplified

Low-collisionality kinetic transport equation:

$$\frac{\partial F_{0f}}{\partial t} + \frac{1}{\mathcal{V}'}\frac{\partial}{\partial r}\left(\mathcal{V}'\Gamma_r\right) + \frac{1}{v^2}\frac{\partial}{\partial v}\left(v^2\Gamma_v\right) - C\left[F_{0f}\right] = S\left(r, v\right) \tag{1}$$

If the gyrokinetic equation is a *linear* PDE (valid in two *independent* limits: **energetic** or **trace**), then the fluxes can be rigorously decomposed:

$$\Gamma_r = -D_{rr}\frac{\partial F_{0f}}{\partial r} - D_{rv}\frac{\partial F_{0f}}{\partial v}$$

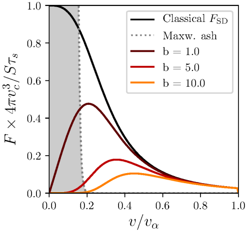
$$\Gamma_v = -D_{vr}\frac{\partial F_{0f}}{\partial r} - D_{vv}\frac{\partial F_{0f}}{\partial v}$$

Wilkie, et al. PoP 2016

- Phase space diffusion coefficients calculated with GS2 gyrokinetic code.
- Eq. (1) solved with the T3CORE phase-space transport code.

Result: radial flattening results in "bump on tail" in energy, along with modest reductions in heating and Alfvén drive.

An analytic transport-modified slowing down distribution



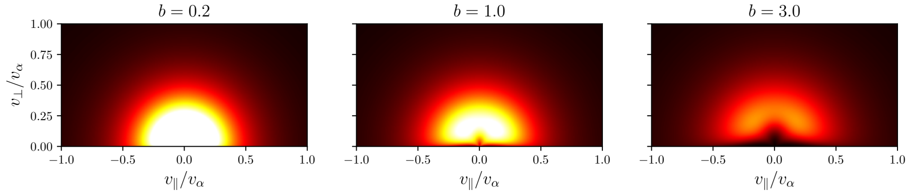
For $D_{rr} \approx D_\alpha \frac{v_\alpha^3}{v^3}$ (Hauff scaling):

$$f_{\mathrm{SD,mod}}(v) = \frac{S_0 \tau_s}{4\pi} \frac{1}{v_c^3 + v^3} \left(\frac{v^3}{v_\alpha^3} \frac{v_\alpha^3 + v_c^3}{v^3 + v_c^3} \right)^{b/3}$$

Dimensionless parameter: $b = \frac{D_\alpha \tau_s}{L_\alpha^2} \frac{v_\alpha^3}{v_c^3}$

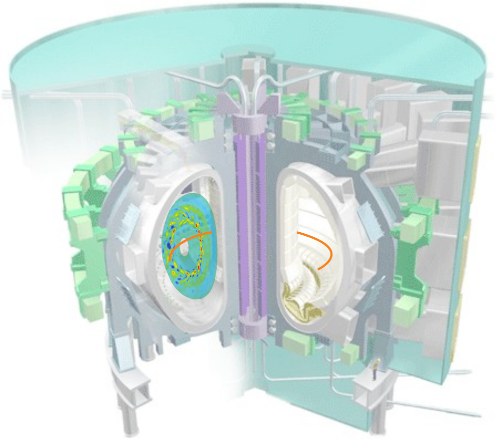
Wilkie. JPP 2018

With pitch angle-dependent transport:



Ashes to ashes: neutral gas to plasma and back again

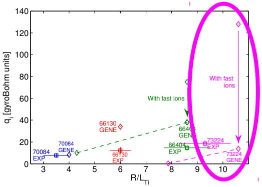
Microturbulence and fast ion stabilization



http://www.itercad.org
Görler, et al. PoP 2011

Fast ions are known to sometimes have a strong impact on plasma microturbulence

- In some JET discharges, the presence of fast ions from NBI and ICRH reduces bulk plasma heat flux by an order of magnitude.
- Not explained by dilution alone.



(Citrin et al. PRL 2013)

Estimate the fast ion contribution to the turbulent fields $\chi = \phi - \left(v_\parallel / c\right) A_\parallel$ from the energetic limit of gyrokinetic for h_f, the non-adiabatic perturbed distribution:

$$v_\parallel \mathbf{b} \cdot \nabla h_f + \mathbf{v_D} \cdot \nabla h_f = -\frac{c}{B} \mathbf{b} \times \nabla \left\langle \chi \right\rangle_{\mathbf{R}} \cdot \nabla F_{0f}$$

$\rightarrow$ a **linear** equation for h_f.

Strong stabilization of ITG turbulence by fast ions and $T_i/T_e > 1$ is the *same physics*

The fast ion contribution to turbulent fields is made especially clear after applying further simplifications:

- Strongly ballooning limit: consider only fluctuations at outboard midplane $\theta = 0$.
- Ignore other impurities.

Wilkie, et al. NF 2018

$$\delta n_f = R_{0f} \frac{e n_e}{Z_f T_i} \phi \qquad \delta j_{\parallel f} = R_{2f} \frac{e^2 n_e}{Z_f T_i} \frac{v_{ti}^2}{c} A_{\parallel}$$

Response functions ($k_y \neq 0$):

$$R_{jf}\left(k_\perp, \eta_f\right) \approx \frac{Z_f^2}{n_e} \frac{T_i}{T_f} \frac{R}{2L_{nf}} \int \left(\frac{v_\parallel}{v_{ti}}\right)^j \frac{1 + \eta_f \left(v^2/v_{tf}^2 - 3/2\right)}{\left(v_\parallel^2 + v_\perp^2/2\right)/v_{ti}^2} J_0^2\left(\frac{k_\perp v_\perp}{\Omega_{0f}}\right) F_{0f} \, \mathrm{d}^3\mathbf{v}$$

Quasineutrality:

$$\frac{e^2}{T_i} \phi \left[\frac{n_i}{n_e} + \tau - R_{0f}\right] = e \frac{\delta n_i}{n_e} = \frac{e}{n_e} \int \left\langle h_i \right\rangle_{\mathbf{r}} \mathrm{d}^3\mathbf{v} \qquad (\tau = T_i/T_e)$$

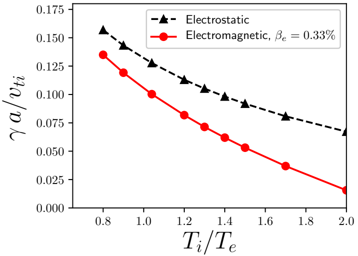
τ_{eff} model predicts all known features of the fast ion stabilization phenomenon

This first-principles reduced model successfully predicts:

τ_{eff} model predicts all known features of the fast ion stabilization phenomenon

This first-principles reduced model successfully predicts:

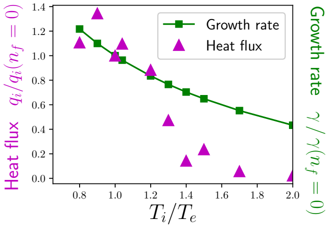
- Disproportionate β stabilization.

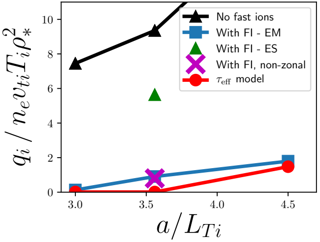


τ_{eff} model predicts all known features of the fast ion stabilization phenomenon

This first-principles reduced model successfully predicts:

- Disproportionate β stabilization.
- Lack of zonal damping leads to strong nonlinear effect. *(Wilkie, et al. NF 2018)*





τ_{eff} model predicts all known features of the fast ion stabilization phenomenon

This first-principles reduced model successfully predicts:

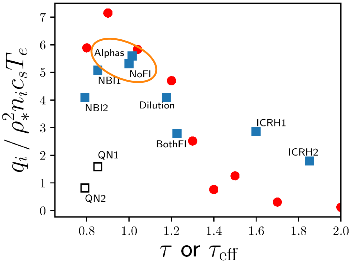
- Disproportionate β stabilization.
- Lack of zonal damping leads to strong nonlinear effect. *(Wilkie, et al. NF 2018)*
- Strong stabilization from auxiliary heating in some discharges; little from alpha particles.

"α-like":

$$n_f = 0.0075 n_e$$
$$T_f = 200 T_i$$
$$a/L_{nf} = 4.5$$
$$a/L_{Tf} = 0.5$$

"ICRH-like":

$$n_f = 0.15 n_e$$
$$T_f = 10 T_i$$
$$a/L_{nf} = 0$$
$$a/L_{Tf} = 5$$

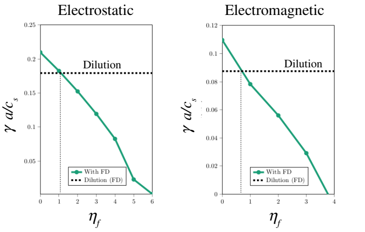


(Wilkie, et al. NF 2018)

$\tau_{\rm eff}$ model predicts all known features of the fast ion stabilization phenomenon

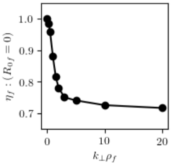
This first-principles reduced model successfully predicts:

- Disproportionate β stabilization.
- Lack of zonal damping leads to strong nonlinear effect. *(Wilkie, et al. NF 2018)*
- Strong stabilization from auxiliary heating in some discharges; little from alpha particles.
- Threshold for pure dilution $\eta_f \approx 0.7 - 1.0$.



(Iantchenko. MSc Thesis 2017)

Threshold η_f from model:



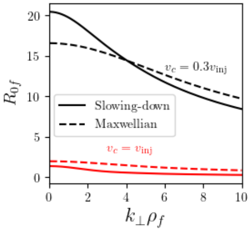
(Wilkie, et al. NF 2018)

τ_{eff} model predicts all known features of the fast ion stabilization phenomenon

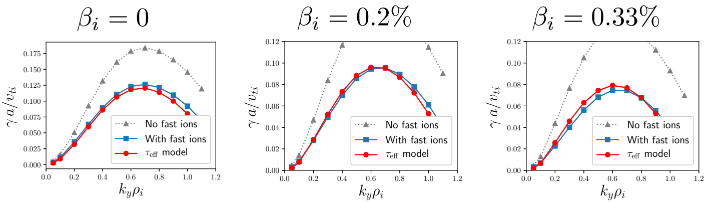
This first-principles reduced model successfully predicts:

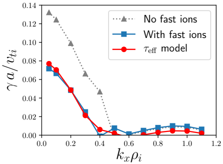
- Disproportionate β stabilization.
- Lack of zonal damping leads to strong nonlinear effect. *(Wilkie, et al. NF 2018)*
- Strong stabilization from auxiliary heating in some discharges; little from alpha particles.
- Threshold for pure dilution $\eta_f \approx 0.7 - 1.0$.
- Stabilization insensitive to non-Maxwellian nature of NBI-like fast ions. *(Di Siena, et al. JoP 2016)*
- Fast ions *destabilize* ETG. *(Bonamoni, et al. NF 2018)*

Response function for slowing-down distribution:

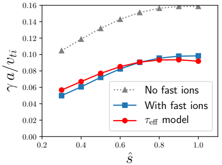


Reduced model is well suited to be used with quasilinear saturation rules





$\tau_{\rm eff}$ model reproduces effect of fast ions for inputs to quasilinear models.



- QuaLiKiz predicts turbulent fluxes from linear physics. *(Bourdelle, et al. PPCF 2016)*
- With lots of simulation-generated data, neural networks are trained for *real-time* transport predictions. *(Citrin, et al. NF 2015)*

Ashes to ashes: neutral gas to plasma and back again

Transport through pedestal and separatrix

- Comprehensive simulation

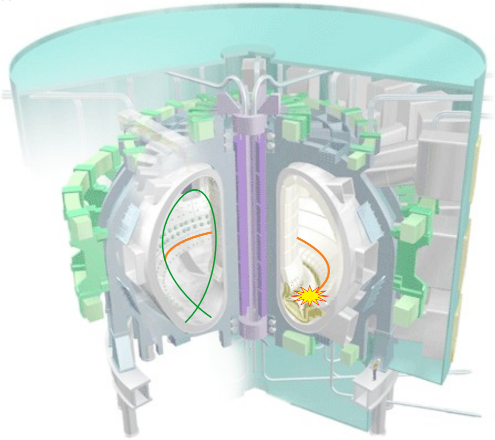
  Churchill, et al. PPCF 2017
- Neoclassical theory

  Chang, Ku & Weitzner. PoP 2004

  Landreman, et al. PPCF 2014
- Local gyrokinetics

  Hatch, et al. NF 2017
- New reduced models

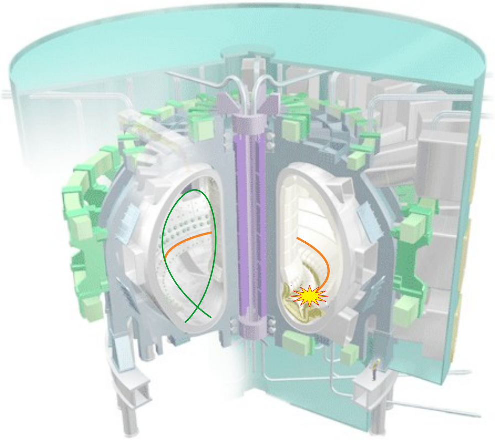
  Abel & Hallenbert. JPP 2018



http://www.itercad.org

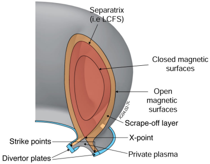
Ashes to ashes: neutral gas to plasma and back again

Recombination at divertor



http://www.itercad.org

Divertors limit exposure of the plasma to solid material

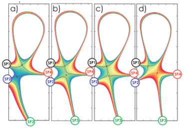


- **Advantage**: low plasma impurity contamination.
- **Disadvantage**: escaping hot plasma strikes a limited surface area.

- Heuristic scaling predicts unfavorable scaling of scrape off layer widths with increasing current. *(Eich, et al. PRL 2011; Goldston. NF 2012)*
- The scrape-off layer width in ITER restricts accessible parameters for high performance discharges, though XGC simulations predict goals still achievable. *(Chang, et al. NF 2017)*
- Close attention must be paid beyond ITER. A solution is needed. . .

Divertors need to be improved for burning reactor

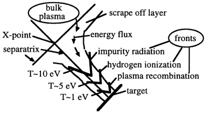
Advanced divertor configurations



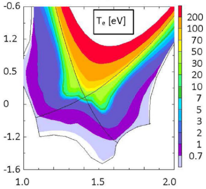
Spreads flux over wider area.

(Labit, et al. Nuc. Mat. & Energy 2017)

Detached divertors:



(Krasheninnikov, et al. J. Nuc. Mat. 1999)

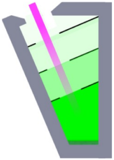


(Krasheninnikov, et al. PoP 2016)

- A regime of operation exists where the wall is shielded from the narrow directed plasma by a layer of neutral gas,
- Situation is unstable and difficult to control: ionization front tends to either falls back to the wall or the plasma.
- Dynamics of neutrals and the gas-plasma transition are important.

Lithium vapor boxes

A novel concept for detachment.



(Goldston, et al. Nuc. Mat. & Energy 2017)

(Emdee, et al. Nuc. Mat. and Energy 2019)

Tools for modelling neutrals in scrape-off layer/divertor

- **Fluid approximation** (e.g., BOUT++). Cheap, but formally only valid for high collisionality.
- **Particle simulation** (e.g., DEGAS2). Comprehensive and rigorous, but expensive to minimize noise in resolving velocity distribution.
- **Hybrid models**
  - Kinetic neutrals with simplified collision operator. *(Wersal & Ricci, NF 2015)*
  - Eulerian time-advance, Monte Carlo calculation of integrals. *(L. Vialetto - DIFFER)*
- **Grid-based methods** (e.g. BOLSIG+). Either too expensive or assumptions too restrictive.

Issue for most methods: **nonlinear neutral-neutral collisions**: more important in high-performance devices with gaseous divertors.

Solving the full nonlinear Boltzmann equation is typically very expensive

$$\frac{\mathrm{d}f_s(\mathbf{v})}{\mathrm{d}t} = \sum_{s',k} \int\int |\mathbf{v}-\mathbf{w}|\sigma_k\left(\mathbf{v},\mathbf{w}\right)\left[\frac{1}{\alpha_k^2} f_s\left(\mathbf{v}'\right) f_{s'}\left(\mathbf{w}'\right) - f_s\left(\mathbf{v}\right) f_{s'}\left(\mathbf{w}\right)\right] \mathrm{d}^3\mathbf{w}\,\mathrm{d}^2\Omega$$

- Choose a discretization: f represented by N degrees of freedom: f_i (particle samples, values on a 3D mesh, spectral coefficients, etc.).
- Because the Boltzmann equation is **quadratically nonlinear**, we can write a discretization scheme for the collision operator as:

$$\frac{\partial}{\partial t}\mathbf{f} = \mathbf{f}\cdot\mathbb{C}\cdot\mathbf{f} \quad ; \quad \frac{\partial}{\partial t} f_p = \sum_{q=1}^{N}\sum_{r=1}^{N} f_q f_r C_{pqr}$$

  where $\mathbb{C}$ is a $N\times N\times N$ **collision hypermatrix**, which is *independent* of the distribution function.

Suppose we attempt to solve on a finite-difference velocity space grid and trapezoidal quadratures with $N = 30^3$ grid points.

- $\sim 10^{18}$ operations to calculate the ~ 4 TB collision matrix.

A spectral expansion for the Boltzmann equation

1. Expand distribution function in an orthonormal basis:

Gamba & Rjasanow. JCP, 2018

$$f(\mathbf{v}) \approx \sum_{k,l,m} f_{klm}\phi_{klm}(\mathbf{v})$$

$$= \sum_{k,l,m} f_{klm}\sqrt{\frac{2k!}{\Gamma(k+l+3/2)}}e^{-v^2/2}v^l L_k^{l+1/2}\left(v^2\right)Y_{lm}(\theta,\phi)$$

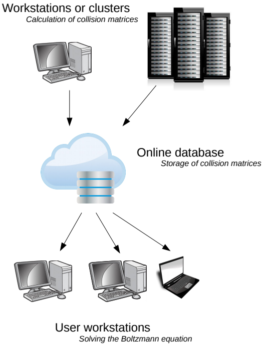
2. Solve the **weak form** of the Boltzmann equation. Multiply through by a *test function* ψ and integrate over all $\mathbf{v}$.

$$\psi_{klm}(\mathbf{v}) \equiv v^l L_k^{l+1/2}\left(v^2\right)Y_{lm}(\theta,\phi)$$

Each of the N^3 elements of $\mathbb{C}$ is an 8-dimensional integral. Need to be as efficient as possible.

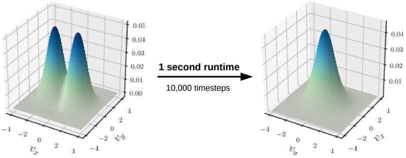
- Use Lebedev quadrature for solid angle and efficient Gaussian quadrature tailored to the Maxwellian distribution and/or collision cross section. *(Wilkie, PhD thesis. 2015)*

LightningBoltz is a new and expanding tool for solving the nonlinear Boltzmann equation



- Optimized, parallelized, and rigorously benchmarked.
- Manifestly conserves collisional invariants.

Single CPU performance:



- Extends the Galerkin-Petrov algorithm for:
  - Inelastic collisions.
  - Improved Gaussian quadrature.
  - Force field acceleration
  - Linear collision operators
  - Implicit time advance

Proof of principle: neutral collisions, excitation, and reactions

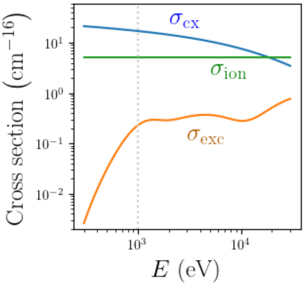
LightningBoltz can handle inelastic, nonlinear, and transformative collisions

$$\frac{\partial f_n}{\partial t} = n_e \alpha_{\rm recom} f_i - n_e \left\langle v \sigma_{\rm ion} \right\rangle_e f_n + C_{\rm el}\left[f_n, f_n\right] + C_{\rm inel}\left[f_n, f_n\right]$$

"Proof of principle" model

- $C_{\rm el}\left[f_n, f_n\right] \approx$ Elastic proton charge exchange
- $C_{\rm inel}\left[f_n, f_n\right] \approx$ Proton impact excitation
- $\alpha_{\rm recom} =$ Radiative recombination
- $\sigma_{\rm ion} =$ Electron-impact ionization

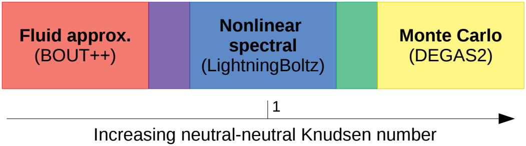
Janev, Reiter, Samm. 2003.



Can also read from LXCat and Open-ADAS files. (in progress)

Where do spectral schemes fit in the modelling of neutrals?

- Being extremely efficient, much simulation data can be generated.
- Machine learning can be used to:
  - Inform comprehensive DEGAS2 simulations about neutral-neutral collisions
  - Generate a neural network-based *closure* for fluid models.
  - Develop real-time predictive capability for detachment control systems.
- Couple to DEGAS2 for the transition to fluid-like behavior.



Conclusion

- From initial formation inside the neutral beam injector to radiator in the divertor region, a neutral atom/ion encounters many phenomena that that are computationally intensive to predict.
- Reduced models, informed by comprehensive HPC simulations, can be used to reduce computational cost and improve physical understanding.
- Solving the transient Boltzmann equation is feasible on modern workstations without assumptions (apart from discretization).

Thank you to collaborators:

I. Abel, A. Iantchenko, E. Highcock,
I. Pusztai, T. Fülop, W. Dorland,
M. Landreman, F. Parra

Further reading:

- Wilkie, et al. "First principles of modelling the stabilization of turbulence by fast ions." *Nuclear Fusion* (2018)
- Wilkie, et al. "Transport and deceleration of fusion products in microturbulence." *Physics of Plasmas* (2016)
- Wilkie. "Analytic slowing-down distributions as modified by turbulent transport." *Journal of Plasma Physics* (2018)
- Gamba & Rjasanow. "Galerkin-Petrov approach for the Boltzmann equation." *Journal of Computational Physics* (2018)